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Part 2 of 2

SCALE MODEL ULTRASONIC STUDY OF ARCTIC ICE

by

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December 1979

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Description of a computer program to calculate the mode structure of an ice plate floating on water. Reflectivity of sonic signals which set up modes is used to determine the thickness of the reflecting ice plate.

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Preface

This Final Report contains the M.S. Thesis of Mr. Douglas Himberger, submitted for publication December 1979. The work describes the mathematical background and the physical principles which were used to perform calculations of sonic reflectivity from the water side of a water-ice-air layered system where the angle of incidence is varied to produce changes of the magnitude and the phase of the incident sonic beam as it is reflected from the ice. It is shown that evaluation of these changes in reflectivity can be used to determine the thickness of the ice without having to be in direct mechanical contact with the ice.

The computation of modulus and phase of the reflected beam is accomplished via a modified Simplex Computation Method. The basic concepts of the method are described, as are the modifications incorportated to make the program useful for calculations of ice thicknesses which one would ordinarily expect to encounter in the Arctic Ocean.

The Report shows that there are ranges of angle of sonic incidence and ranges of the expected product ice thickness times sonic frequency where the results of reflectivity measurements are sufficiently characteristic so that variations in the mechanical properties of the ice (as for instance, longitudinal and shear wave propagation velocities) influence the interpretation of the results to a negligible extent so that an assessment of the ice thickness is in principle possible for any kind of ice. It is also pointed out in which ranges of angle of incidence and sonic frequency times expected ice thickness the results of reflectivity measurements will depend highly on a previous knowledge of the mechanical properties of the ice, i.e., which ranges should be avoided.

Examples of calculations and some experimental measurement points are given to illustrate the usefulness of the technique. A complete computer program is given which can be used to calculate any combination of parameters of interest. A number of figures are presented to illustrate the influence of changes in the parameters on the relfectivity results and thus on the degree of reliability of thickness measurements.

Walter G. Mayer

Principal Investigator

Washington, D.C., December 1979

CHAPTER 1

INTRODUCTION

Knowledge of the propagation characteristics of sound waves, particularly of those in the ultrasonic region, is critical in many areas of scientific research. Notable fields among these are seismic studies, nondestructive testing, and sonar detection. An evaluation of sound reflection from and/or transmission through a particular medium may reveal information about a number of physical parameters of that medium. One of these parameters is the thickness of a solid reflector bounded by a liquid. Firestone [1] observed that a sound wave impinging on a flat solid plate, immersed in a liquid, will be reflected or transmitted depending on the angle of incidence. Maximum transmission will occur if the incident sound wave excites a normal mode of vibration of the plate. These normal modes of vibration were described by Lamb [2] who found that the number of possible modes and their propagation velocities are determined by the elastic properties of the solid, the frequency of excitation, f, and the thickness of the plate, d. Experimentally [3], the mode structure does not change significantly if one considers a solid plate vibrating in a vacuum (the approach used by Lamb) or in a fluid as long as the density of the solid is at least three or four times greater than the density of the surrounding medium.

Huang [4] developed a set of formulas which show that the mode

structure changes significantly when the solid plate is bounded by a liquid on one side and air on the other. Of particular interest is the case where such an asymmetric loading exists and where the density of the solid is less than the density of the liquid. An example of such a system is an ice sheet floating on water. Since the ice sheet exhibits normal modes of vibration when excited by an underwater acoustic wave, it is conceivable that one can determine the thickness of the ice from the results of reflectivity measurements at various angles of incidence.

This thesis presents a method of determining computationally the reflectivity as a function of angle of incidence for a three layer, three substance system, specifically for the air/ice/water subsystem. Calculations are presented for an fd (frequency-thickness product) range up to 4×10^6 Hz·mm.

CHAPTER II

BACKGROUND

The basic starting point for the study of sound reflectivity characteristics is the analysis of the behavior of sound impinging on a flat interface between two differing substances. In general, a sound wave (or beam) incident at a flat interface obeys the law of specular reflection; that is, the angle of reflection is equal to the angle of incidence. However, there are several instances [5] where this does not hold true. In addition to the wave being reflected specularly (and being transmitted to some degree), a surface wave may be set up in the solid for several angles of incidence (assuming one of the layers is a solid). These are waves that propagate along the interface between the solid and the liquid. These "leaky" surface waves are attenuated as they re-radiate energy back into the liquid. The generation of leaky surface waves at these special angles of incidence gives rise to an unusual type of reflection, known as "non-specular", and gives an indication that the other parameters of the system (thickness, frequency) are in a particular arrangement. To determine when these special reflections occur, one must first find a functional description of the reflection and solve for zero reflection (maximum transmission).

The most simple system, which Lord Rayleigh [6] studied, is one of an infinitely thick solid plate bounded by a vacuum. He determined that the solid can support one surface wave, the Rayleigh wave. How-

ever, this surface wave cannot be excited by an incident beam as there is no medium to propagate such a sound beam to the solid.

Because it was shown to have similar vibrational modes [3], the next system to consider is that of an infinitely thick plate bounded by some liquid. Schoch [5] and Brekhovskikh [7] studied sonic reflection at the interface formed by this liquid/solid system (or L/S system) and reported non-specular reflections. Figure 1 shows the law of specular reflection for the incident beam and the transmission of part of the beam by both shear and longitudinal waves in the solid. The directions of propagation of the various waves can be found from Snell's law, given by

$$\frac{\sin \theta_\iota}{v_\iota} = \frac{\sin \theta_d}{v_d} = \frac{\sin \theta_s}{v_s} \quad (1)$$

where ι denotes liquid, s denotes shear, and d denotes longitudinal. For most liquid/solid systems the magnitudes of the velocities are related by the inequality $v_d > v_s > v_\iota$. Using these facts and the formalism of Pitts [8], one can arrive at a reflection coefficient (a ratio of the amplitudes of the reflected wave and the incident wave) as a function of the angle of incidence and the densities of the liquid and the solid. The reflection coefficient, as formulated by Pitts, is given by

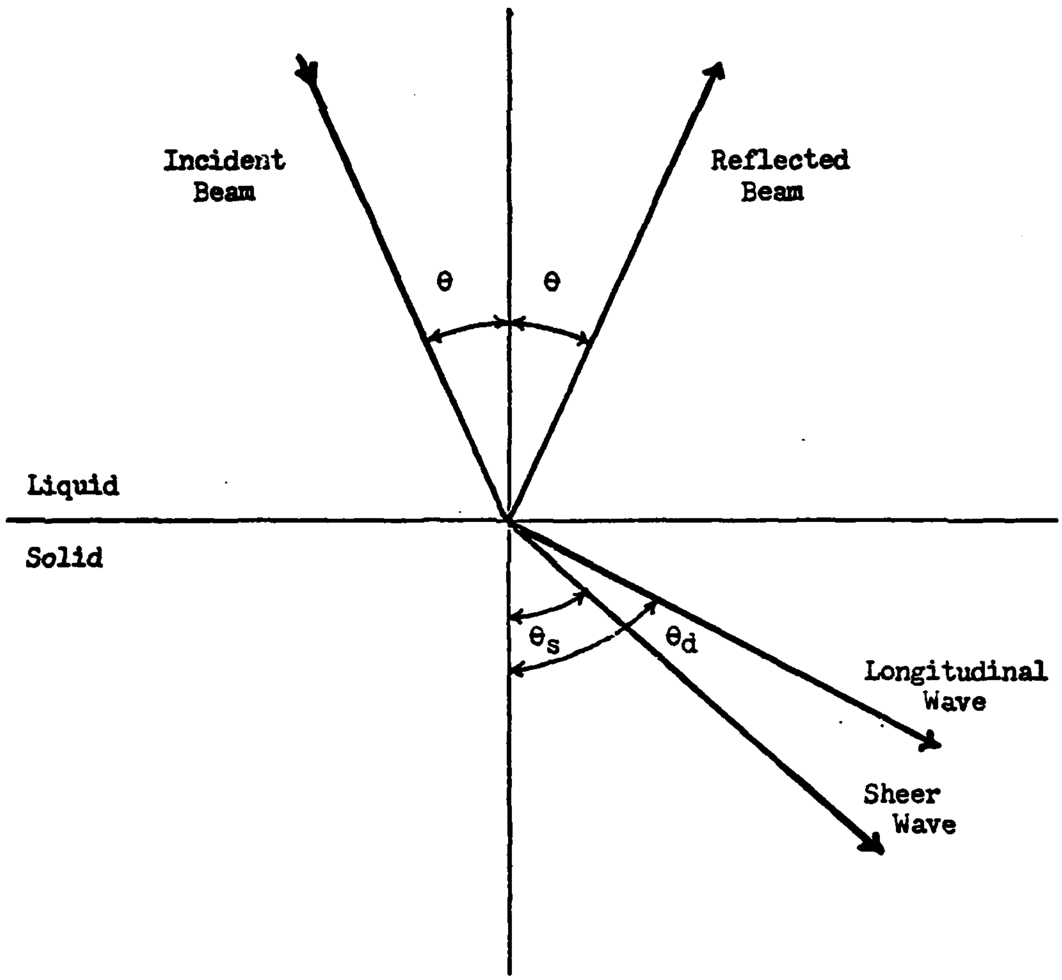

Figure 1 -- Reflection and transmission of sound wave at a liquid/solid interface.

$$R(k_x) = \frac{(k_s^2 - 2k_x^2)^2 + 4k_x^2 K_s K_d - \rho k_s^4 K_d / K}{(k_s^2 - 2k_x^2)^2 + 4k_x^2 K_s K_d + \rho k_s^4 K_d / K} , \qquad (2)$$

where the following definitions are used

k = wave number,

$$K = k_\iota \cos\ \theta = k\sqrt{1-\sin^2\ \theta}\ , \qquad (3)$$

$$K_s = k_s \cos\ \theta = k\sqrt{(v_\iota/v_s)^2 - \sin^2\ \theta}\ , \qquad (4)$$

$$K_d = k_d \cos\ \theta = k\sqrt{(v_\iota/v_d)^2 - \sin^2\ \theta}\ , \qquad (5)$$

θ = angle of incidence ,

ρ = density of liquid/ density of solid. (6)

Equation (2) has a zero for a specific angle of incidence (in a system where all other parameters are defined). It is at this angle where a surface wave, the leaky Rayleigh, can be excited. There are, however, certain systems, as found by Brower, Himberger, and Mayer [9], where this solution may not exist due to certain combinations of v_ι , v_s , v_d , and ρ. For the systems where a solution does exist, a simple scan or search method would be sufficient to solve for the zero. The function is also simple enough that a type of gradient or derivative method could be used (this type of method's use depends on the ease with which the function's derivative can be found).

The system becomes more complicated when the solid is made to be of finite thickness and is loaded on both sides by a liquid, in which

case two boundaries must now be considered. Figure 2, taken from Pitts [8], shows this situation in terms of the previously defined quantities. The coefficient formulated by Pitts [8] for this system is given by

$$R(k_x) = N/(f_s f_a) \tag{7}$$

where

$$f_s = (k_s^2 - 2k_x^2)^2 \frac{(1 + \cos P)}{\sin P} + 4k_x^2 K_s K_d \frac{(1 + \cos Q)}{\sin Q} - \frac{i\rho\, k_s^4 K_d}{K} , \tag{8}$$

$$f_a = (k_s^2 - 2k_x^2)^2 \frac{(1 - \cos P)}{\sin P} + 4k_x^2 K_s K_d \frac{(1 - \cos Q)}{\sin Q} - \frac{i\rho\, k_s^4 K_d}{K} , \tag{9}$$

$$N = (k_s^2 - 2k_x^2)^4 + 16k_x^4 K_s^2 K_d^2 - \rho^2 k_s^8 K_d^2/K^2 + 8(k_s^2 - 2k_x^2)^2 k_x^2 K_s K_d (1-\cos P\cos Q)/(\sin P\sin Q), \tag{10}$$

$$P = d\, k_d \cos \theta_d , \tag{11}$$

$$Q = d\, k_s \cos \theta_s , \text{ and} \tag{12}$$

d = thickness of plate.

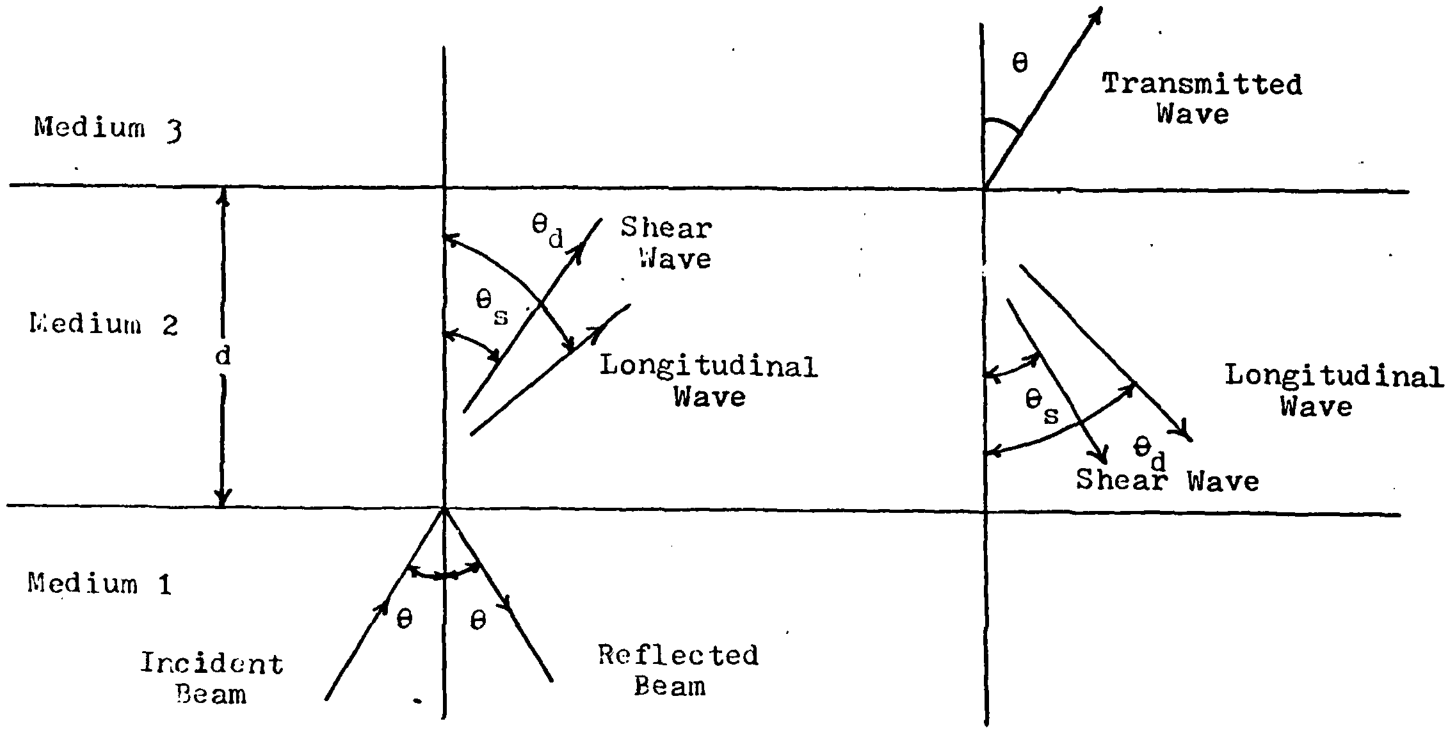

Figure 2. Reflection and refraction of sound at a liquid/solid/liquid interface.

The relationship between the angle of incidence, θ, and the thickness of the solid plate is complicated. This situation requires a more sophisticated type of optimizing technique.

One finds several zeroes for (7) for a given fd or angle of incidence. These solutions correspond to the modes of vibration the incident beam is capable of exciting in the solid plate. An example system is the water/brass/water system of Pitts [8]. Figures 3 and 4 show the real part of the zeroes of the f_s and f_a terms for different fd's and incident angles. Although solutions to these terms, equations (8) and (9), represent solutions to the denominator of the reflection coefficient, and thus are poles, it has been shown [8] that the solutions to the numerator (the zeroes) have the same real sin θ value. It has also been shown [8] that these pole-zero pairs are complex conjugates of each other when the imaginary part is also included. It is, however, the real part of the angle that will be measured when a non-specular reflection is observed. The curves in figs. 3 and 4, taken from Pitts [8] , are referred to as modes, representing the modes of vibration of the solid plate.

The relation given by (7) becomes more complicated when one goes to an even more general system in which the plate is surrounded by two dissimilar fluids, or by a fluid and a gas, as in the air/ice/water case. There is no distinction between "symmetric" and "anti-symmetric" solutions to the reflection coefficient (Pitts' solutions to the f_s and f_a terms respectively) because neither the system nor the coeffi-

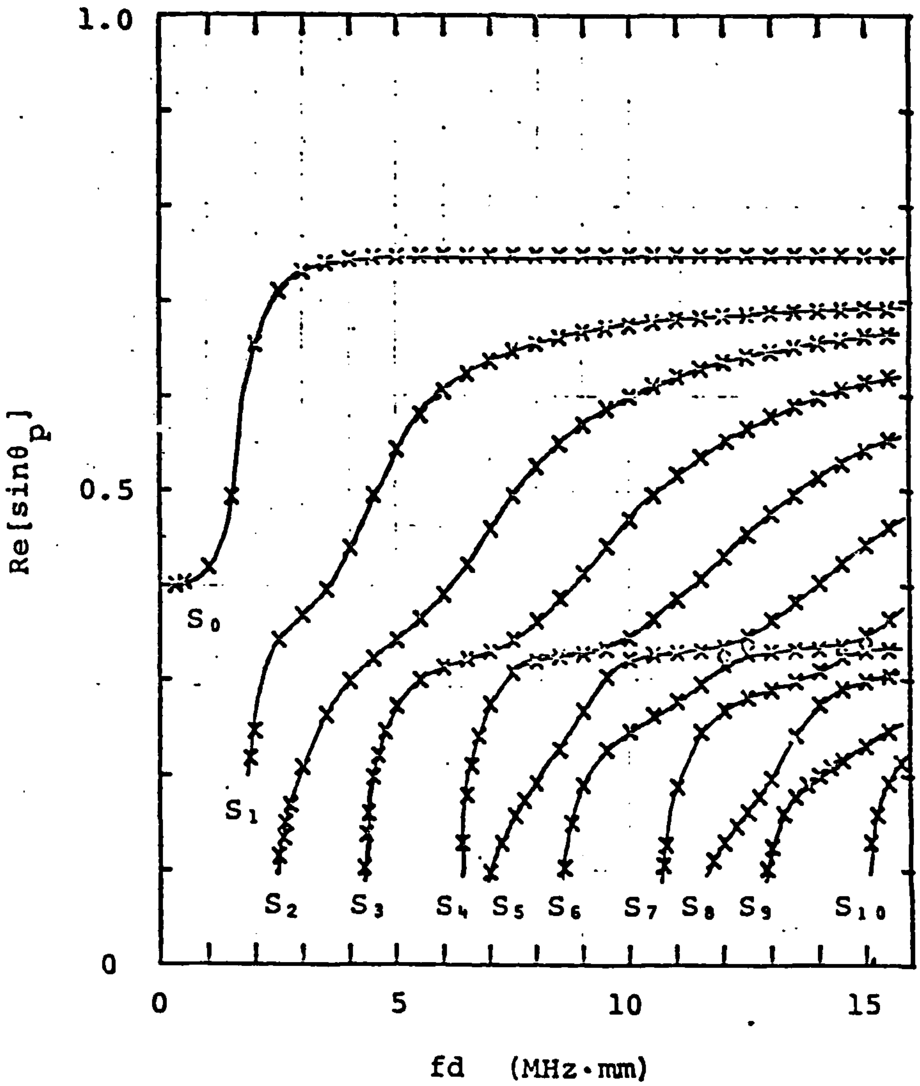

Figure 3. The real part of the symmetric poles of the reflection coefficient in the complex sinθ plane for a brass plate in water as a function of fd. (After Pitts [8])

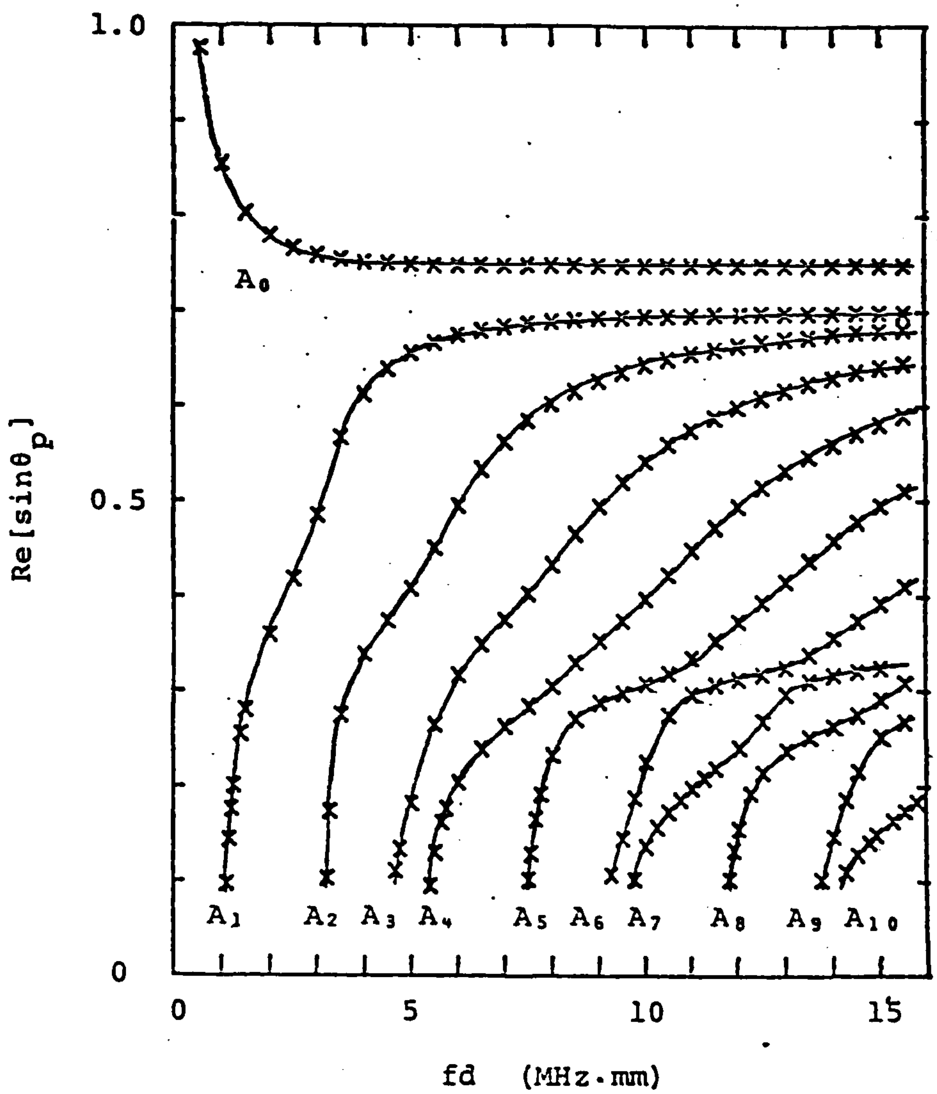

Figure 4. The real part of the antisymmetric poles of the reflection coefficient in the complex $\sin\theta$ plane for a brass plate in water as a function of fd. (After Pitts [8])

cient are symmetric. One can no longer break up the coefficient into two simple terms and find the zeroes for each of these terms. The entire equation must be solved simultaneously. From Huang [4], the coefficient for this type of system is given by

$$R = N/D \quad , \tag{13}$$

where

$$N = A(B-C) + (E+F)G \quad , \tag{14}$$

$$D = A(B+C) - (E-F)G \quad , \tag{15}$$

and

$$A = 2\{ \Omega - [F(\sin\{ \pi fd/v_1[(v_1/v_d)^2 - \sin^2 \theta]^{1/2} \}) \cdot$$

$$(\sin\{ \pi fd/v_1[(v_1/v_s)^2 - \sin^2 \theta]^{1/2} \})]\} \quad , \tag{16}$$

$$B = \{1-2[(v_s/v_1)\sin\theta]^2\}^2 \sin\{ \pi fd/v_1[(v_1/v_d)^2 - \sin^2\theta]^{1/2}\} \cdot$$

$$\cos\{ \pi fd/v_1[(v_1/v_s)^2 - \sin^2\theta]^{1/2}\} +$$

$$\{4[(v_s/v_1)^4\sin^2\theta][(v_1/v_d)^2-\sin^2\theta]^{1/2}[(v_1/v_s)^2-\sin^2\theta]^{1/2}\} \cdot$$

$$\cos\{ \pi fd/v_1[(v_1/v_d)^2-\sin^2\theta]^{1/2}\} \sin\{ \pi fd/v_1[(v_1/v_s)^2-\sin^2\theta]^{1/2}\} \quad , \tag{17}$$

$$C = E \cos\{\pi fd/v_1[(v_1/v_d)^2-\sin^2\theta]^{1/2}\}\cos\{ \pi fd/v_1[(v_1/v_s)^2-\sin^2\theta]^{1/2}\} \quad , \tag{18}$$

$$E = i\ (\rho_1/\rho_2)\ \{[(v_1/v_d)^2-\sin^2\theta]^{1/2}/(1-\sin^2\theta)^{1/2}\} \quad , \tag{19}$$

$$F = i\ (\rho_3/\rho_2)\ \{[(v_1/v_d)^2-\sin^2\theta]^{1/2}/[(v_1/v_3)^2-\sin^2\theta]^{1/2}\} \quad , \tag{20}$$

$$G = \{1-2[(v_s/v_1)\sin\,\Theta]^2\}^2\ \sin\{\pi fd/v_1[(v_1/v_s)^2-\sin^2\Theta]^{\frac{1}{2}}\}\ \cdot$$

$$\cos\ \{\pi fd/v_1[(v_1/v_s)^2-\sin^2\Theta]^{\frac{1}{2}}\}\quad +$$

$$4[(v_s/v_1)^4\sin^2\Theta][(v_1/v_d)^2-\sin^2\Theta]^{\frac{1}{2}}[(v_1/v_s)^2-\sin^2\Theta]^{\frac{1}{2}}\ \cdot$$

$$\sin\ \{\pi fd/v_1[(v_1/v_d)^2-\sin^2\Theta]^{\frac{1}{2}}\}\ \cos\ \{\pi fd/v_1[(v_1/v_d)^2-\sin^2\Theta]^{\frac{1}{2}}\}\quad , \tag{21}$$

$$\Omega = \{1-2[(v_s/v_1)\sin\,\Theta]^2\}^2\ \cos\ \{\pi fd/v_1[(v_1/v_d)^2-\sin^2\Theta]^{\frac{1}{2}}\}\ \cdot$$

$$\sin\{\pi fd/v_1[(v_1/v_s)^2-\sin^2\Theta]^{\frac{1}{2}}\}\quad +$$

$$4[(v_s/v_1)^4\sin^2\Theta][(v_1/v_d)^2-\sin^2\Theta]^{\frac{1}{2}}[(v_1/v_s)^2-\sin^2\Theta]^{\frac{1}{2}}\quad , \tag{22}$$

v_1 = velocity in medium 1 (liquid or gas) ,

v_3 = velocity in medium 3 (liquid or gas) ,

ρ_1 = density of medium 1 ,

ρ_2 = density of medium 2 (solid) ,

ρ_3 = density of medium 3 .

Equations (16) through (22) are expressed on terms of velocities rather than wave numbers as in (2), (8)-(12). Optimizing (13) requires more than a simple technique.

The air/ice/water system is a special case of an L/S/L system because v_l and v_s may be related by

$$v_s > v_l \quad , \quad \text{(in most cases)}$$

$$v_s \leq v_l \quad , \quad \text{(in rare cases)}$$

where again v_l refers to the sound velocity in the water and v_s refers to the shear velocity in the ice. Clearly, the sound velocity in air is always less than v_s. Moreover, this system differs from most L/S/L systems because the density of the solid is less than that of the loading liquid (ρ_{ice} =0.917, ρ_{water} =1.02).

Although the shear wave velocity in the ice may be less than the sound velocity in water [10], the present paper is concerned only with L/S/L systems where $v_s \geq v_l$, the more common situation.

A computational method, the simplex, was adapted to solve (13) representing this complicated general system. The interpretation of the results then determined the feasibility of finding the thickness of an ice layer by observing the variations in the reflection as a function of sonic frequency and angle of incidence.

CHAPTER III

THE SIMPLEX

To solve the reflection coefficient expressed by (13) in the most efficient and flexible manner, five methods were investigated: the Newton-Raphson gradient method [11], the Rosenbrock direct-search method [12], the Powell 'sum of squared residuals' method [13], the Powell direct search method [14], and the Nelder and Mead simplex direct search method [15].

One of these minimization techniques was excluded from consideration as a result of initial investigation. The Newton-Raphson (and others similar to it, such as the Fletcher-Powell method [16]) is a gradient method which requires that not only the function itself be defined but also the derivative of the function be known. For many functions this is not a problem, but upon close inspection one sees that (13) does not appear to lend itself to this type of technique because of the complexity of the function and the difficulty of finding its derivative.

Powell's 'squared residual' optimization technique (and others with similar characteristics such as Barnes' method [17]) does not require that the derivative of the function be known. While this is an advantage in many cases, Powell's method is not suited for all functions. Box [18] states, "It may not be possible to reformulate every optimization problem as the solution of a set of simultaneous equa-

tions [which Powell's method requires for the 'squared residuals']. . . Certainly it is often not feasible to attempt this." It is unlikely that (13) could easily be separated into the desired set of equations. For a complicated function, Box [18] states, "It has been known for the computation of all residuals for a single set of parameter values to take up to 1,000 times as long as the organization of the search." Even if the set of equations necessary for Powell's method was available, the factor of computation time would remove this type of technique from consideration.

Some type of 'direct search' method is more likely to minimize (13) without the problems associated with the previous methods discussed. The direct search methods investigated were Rosenbrock's [12], Powell's [14], and Nelder and Mead's [15].

Kowalik and Osbourne [19] compare Nelder and Mead's method, the simplex, to Rosenbrock's method and state the two methods have "comparable efficiency when tested on problems with a small number of independent variables. . . however, . . .[for some specific functions] the Simplex method has shown superiority over [Rosenbrock's method]". Kowalik and Osbourne also agree with Nelder and Mead in the latters' evaluation that the simplex method held an advantage over Powell's method in having a faster convergence for several example functions. In addition, should the function have two or more solutions within close proximity, Nelder and Mead state that the simplex "will converge even when the initial simplex straddles two or more valleys,

a property which is not shared by, e.g., Powell's method." Because the forms of the modes (the solutions) of (13) are not known, the ability of the method to converge regardless of the initial guess is useful. The simplex method, in Nelder and Mead's words, is "highly opportunist, in that the least possible information is used at each stage and no account is kept of past positions. No assumptions are made about the surface except that it is continuous and has a unique minimum in the area of the search." In addition, the simplex method, according to Nelder and Mead, is "computationally compact". For all of the above reasons, the simplex was chosen as the minimizing technique to solve for the zeroes and poles of (13).

The simplex method of optimization was developed by Himsworth, Spendley and Hext [20]; it was later studied in detail by Nelder and Mead [15]. Although the technique was originally developed for use in business and economics (plant management, etc.), the method was used in mathematics and science fields to some degree in the early 1960's. Its use in technical fields has decreased however, and today the method is utilized almost exclusively by the business world.

The simplex is a 'steep ascent' method that needs no derivatives and simply forms a geometric figure, the simplex (from which its name is derived), and calculates the actual functional value at the vertices of this figure. The definition of a simplex is given below as a direct quote from Kowalik and Osbourne [19];

". . .a set of n+1 points in n-dimensional space forms a simplex. When these points are equidistant the simplex is said to be regular." The role of the simplex is to find the minimum of a particular function by "sliding" along the functional value, whether this sliding is done along a one-dimensional line, a two dimensional plane, or a three dimensional surface. The simplex, as stated by Nelder and Mead [15], "adapts itself to the local landscape, elongating down long inclined planes, changing direction on encountering a valley at an angle, and contracting in the neighborhood of a minimum." For added flexibility in finding minima, Nelder and Mead generalized the simplex to make it non-regular, that is, not necessarily regular or symmetric in nature.

The algorithmic process of the simplex is given in fig. 5, taken from Nelder and Mead [15]. The simplex has three basic operations; reflection, expansion, and contraction. The definitions of these operations and of basic terms are given by Kowalik and Osbourne [19] as follows:

"(1) x_h is the vertex which corresponds to $f(x_h) = \max f(x_i)$, where $i=1,2,\ldots,n+1$.

(2) x_s is the vertex which corresponds to $f(x_s) = \max f(x_i)$, where $i \neq h$.

(3) x_ℓ is the vertex corresponding to $f(x_\ell) = \min f(x_i)$, where $i=1,2,\ldots,n+1$.

(4) x_o is the centroid of all x_i, $i \neq h$ and is given by

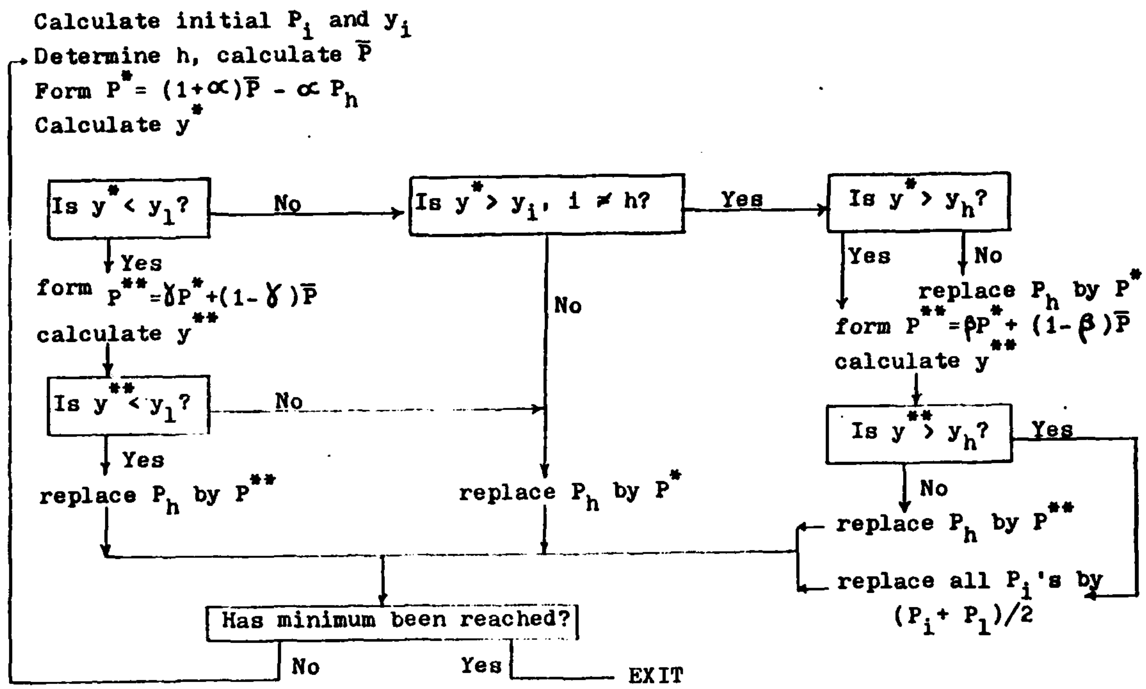

Figure 5 -- Flow diagram of simplex routine. P=parameter value, y=function value, *-indicates reflection, **-expansion or contraction, $\overline{P}$=centroid of points, $i \neq h$, and α, γ, β, are constants.

$$x_o = \frac{1}{n} \sum_{\substack{i=1 \\ i \neq h}}^{n+1} x_i$$

We now define the three basic operations used in the method:

(1) Reflection, where x_h is replaced by

$$x_r = (1 + \alpha)x_o - \alpha\, x_h,$$

where the reflection coefficient $\alpha > 0$ is equal to the ratio of the distance $[x_r x_o]$ to $[x_h x_o]$.

(2) Expansion, where x_r is expanded in the direction along which a further improvement of the function value is expected. We use the relation

$$x_e = \gamma x_r + (1 - \gamma)x_o,$$

where the expansion coefficient $\gamma > 1$ is the ratio of the distance $[x_e x_o]$ to $[x_r x_o]$.

(3) Contraction, by which we contract the simplex,

$$x_c = \beta\, x_h + (1 - \beta)x_o,$$

where the contraction coefficient β is the ratio of the distance $[x_c x_o]$ to $[x_h x_o]$ and satisfies $0 < \beta < 1$.

As we have mentioned, the method can be viewed as the moving, shrinking, and expanding progress of the simplex toward the minimum. This motion is accom-

plished in the following way:

(i) An initial simplex is formed, and the function is evaluated at each of the vertices in order to determine x_h, x_s, x_ℓ, and x_o.

(ii)We first try reflection and evaluate the function at the reflected point.

(iii) If $f(x_s) \geq f(x_r) \geq f(x_\ell)$, then we replace x_h by x_r and restart the process with the newly formed simplex.

(iv) However, if $f(x_r) < f(x_\ell)$, we may expect that the direction $x_r - x_o$ could give us an even lower value of the function if we move further. Therefore we expand our new simplex in this direction. The expansion succeeds is $f(x_\ell) > f(x_e)$, and in this case x_h is replaced by x_r, and in either case we restart the process from our new simplex.

(v) If the reflection move (ii) yields x_r such that $f(x_h) > f(x_r) > f(x_s)$, we replace x_h by x_r and make the contracting move. This replacement is not executed when $f(x_r) > f(x_h)$. After the contracting move we compare the $f(x_h)$ and $f(x_c)$. If $f(x_h) > f(x_c)$, we consider that the contraction is successful, x_h is replaced by x_c, and we start from the

new simplex.

In a case of failure, i.e., $f(x_h) < f(x_c)$, the last simplex is shrunk about the point of the lowest function value x_ℓ by the relation

$$x_i = \tfrac{1}{2}(x_i + x_\ell)$$

and we begin from (i).

The stopping criterion suggested by Nelder and Mead is

$$\{ 1/n \sum_{i=1}^{n+1} [f(x_i) - f(x_o)]^2 \}^{\frac{1}{2}} < \varepsilon ,$$

where ε is some small preset number."

CHAPTER IV

MODIFICATIONS OF THE SIMPLEX

The simplex routine was executed in a FORTRAN IV computer program for use on both the IBM 370/148 computer at the Academic Computation Center at Georgetown University and a DEC PDP-MINC 11 system at Harry Diamond Laboratories. FORTRAN was used because of its capacity for handling involved calculations with ease as well as its ability to deal with complex numbers. This was necessary due to the fact that (13) has solutions that are in general complex.

The program itself was based on a simplex program developed by Huang [4] to deal with similar problems; both are derived from Nelder and Mead's flowchart as given in chapter III of this paper.

The functional changes made in Huang's program involve the following parts of the routine;

(i) When no 'new minimum' is reached by a reflection (the operations identified in section (v) of Kowalik and Osbourne, as quoted in chapter III), the new contracted simplex parameters are specified.

(ii) When setting up the initial simplex, the centroid calculation is set as specified by Nelder and Mead [15].

These changes in Huang's program made the new simplex routine both computationally faster and numerically more consistent. The number

of iterations needed to reach the minimum of a test function was reduced from an average of 150 to 80. The minimum found in the test function was consistent to five decimal places even when the iteration was begun at several different starting points.

Nelder and Mead [15] state that a "general problem encountered by all minimization methods is that of false convergence at a point other than the minimum. This difficulty has been found using the simplex method...". It is because of these 'false minima' that the ability to trace a mode, such as one similar to those in figs. 3 and 4, becomes important. Lacking this ability, it would be difficult to differentiate between local minima and the physically meaningful solutions. Several features were added to the simplex which remove this difficulty. The first was a set of signal 'flags' telling the investigator what series of reflections, contractions, etc. of the simplex were used to reach a final minimum. This was done in order to predict to which minimum the simplex would iterate from a given starting point.

Secondly, the program was put into two separate forms; a concise, simple 'scan' of a given fd for all values of sin Θ, and a rigorous mode-tracing form that not only followed a particular mode but gave information about adjacent modes. The first form was used to find the starting points of any and all modes for a set of parameters and the second was used to generate full sets of curves for these parameters.

Several special features were added to the mode-tracing form. Though the simplex inherently samples the function's three dimensional

space (in the present case these dimensions being the product fd, the value of sin θ, and the functional value for any of these two parameters) until it finds a valley into which to go, the new form of the simplex was 'forced' to search in a given volume of a suspected minimum even if another mode was nearby. While this search was in progress, other minima found (or even tended towards) were indicated in the output so that a better knowledge of the function in the three dimensional space under scrutiny would be gained. When dealing with the beginning of the mode in question, this range of forced iteration was determined by the initial fd scan form of the simplex. In following the mode, once a solution was found in the sampling volume, the range of forced iteration was determined by the last point found and a judicious choice of limits set by the operator watching the tracing of the mode.

When the simplex could not iterate to a minimum within the given limit of iterations (determined by the amount of computer time available), the output also included the intermediate value reached so that some information would be gained about a troublesome range of the function. This point could then be re-examined after slightly varying the starting point, the iteration step size, or both.

The function described by (13) varies in such a way as to make the above additions to the simplex useful. For most test functions such as those used by Box [18], Kowalik and Osbourne [19], and this author (during the preliminary simplex testing), no surface around a minimum

had a form that caused the simplex method problems with respect to local minima, adjacent modes, etc. For the function given by (13) however, this was not true. Figure 6 shows two different example minima, each with considerably different approach slopes. If a function varied in a manner shown in fig. 6(b), a small change in the independent variable (in the present case, the fd or sin θ) would cause a great change in the dependent variable (the functional value in the present case). This rapid variance would cause the simplex to miss or 'step over' one mode in favor of another close and more gradually approached mode, such as the one shown in fig. 6(a). When this happened in tracing a mode, a physically meaningful solution was regarded at times as a local minimum. Unfortunately, the form of the solution to the reflection coefficient of the air/ice/water case has many such steep approaches to minima. An example of this 'steep valley' situation is indicated in Table I which represents a zero of the denominator of the reflection coefficient (eq. (13)) when the system has a density ratio of the first liquid to the solid of 0.3 (compared to 1.1 for normal water/ice density ratio), and velocities in ranges similar to the normal air/ice/water case.

Table I. "Steep Valley" variation of function value.

Starting sin θ	Real sin θ	Imag. sin θ	Function Val.
0.540	0.562996	-.0117405	-.568E-06
0.600	0.562996	-.0117408	-.293E-05

v_1=1500 v_s=1550 v_d=3500 v_3=340 fd=0.65 ρ_ℓ/ρ_s=0.3

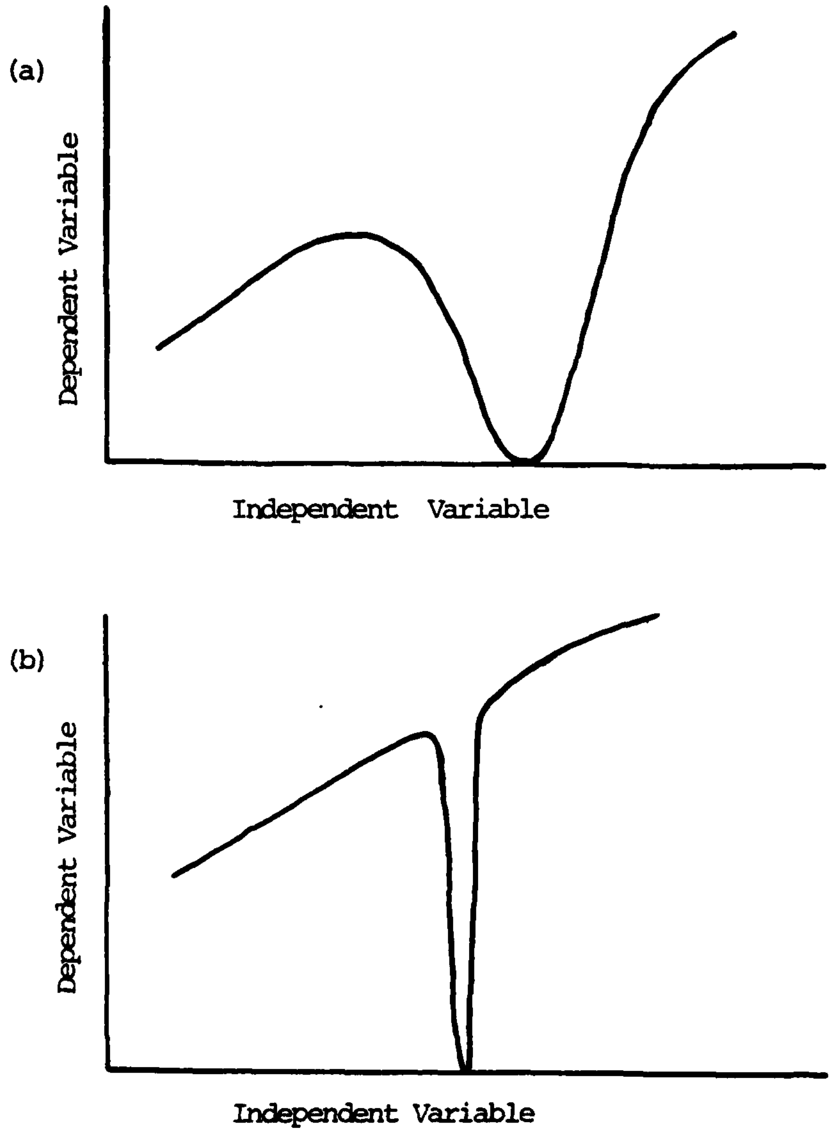

Figure 6. Example of gradually-approached solution to reflection coefficient (a) and steeply-approached solution (b). Ordinate is the independent variable, absissa is the dependent variable.

The approach slope is so steep that when the real parts of sin θ are equal to six places, a change in the sixth decimal place of the imaginary part causes a change in the functional value of one order of magnitude. This solution was missed in both a scan and a mode trace when using the old simplex form.

Besides improving the reliability of the simplex in terms of finding solutions, the additions enable the new form to trace complete modes in one-tenth the time of the old form. This reduction in computation time makes the simplex a reasonable tool for solving complicated functions such as (13). The final form of the simplex mode trace routine is given in Appendix A.

CHAPTER V

RESULTS

A. Two-substance system results.

The modified simplex optimizing technique, as described in chapter 4, was used to solve (13) for parameters of a water/brass/water system, previously described by Pitts [8]. Table II contains the results of the simplex and those of Pitts.

Table II. Water/Brass/Water Reflection Coefficient Poles
(fd = 5)

Pitts		Simplex	
Re(sinΘ)	Im(sinΘ)	Re(sinΘ)	Im(sinΘ)
0.002	0.454	0.290307E-02	0.454711E00
0.004	0.302	0.485337E-02	0.302640E00
0.182	0.0075	0.182645E00	0.751577E-02
0.273	0.0017	0.273108E00	0.177726E-02
0.342	0.0001	0.342847E00	0.995920E-04
0.408	0.0048	0.408948E00	0.487755E-02
0.544	0.0057	0.544637E00	0.578639E-02
0.656	0.0034	0.656149E00	0.347561E-02
0.747	0.0136	0.747784E00	0.136844E-01
0.750	0.0125	0.750331E00	0.125455E-01

The results of the simplex confirm Pitts' original calculations for the water/brass/water system. The results also confirm that (13) re-

duces to (7) when the same liquid bounds the plate on both sides.

B. Three-substance system results.

Values for air, ice and water parameters, given by Sató [10], were substituted in (13) and this function was run in the simplex. Figure 7 shows the results of the runs for the air/ice/water reflection coefficient for fd's of zero to four. The graph shows a general form similar to that of figs. 3 and 4 from Pitts [8]. There are several major differences, however. Two of the modes shown in fig. 7 are not continuous whereas all of the modes in previous studies have been. The modes intercepting the abscissa (representing integer half-wavelength "standing wave" solutions for incoming beams of normal incidence) correspond to the half-wavelengths of the shear wave as expected, but no intercepts representing the longitudinal wave occur. Finally, one of the modes has a definite negative slope, suggesting a negative group velocity. Viktorov [21] anticipated this possibility, but it has not been confirmed. Due to the above differences, several changes were investigated in an effort to clarify the situation.

C. Adjustment of solid density.

Brower, Himberger, and Mayer [9] showed that leaky Rayleigh surface waves cannot be generated on certain systems, specifically the ice/water system. Zeroes of the reflection coefficient are known to have a definite relationship to non-specular reflection and hence to surface waves, Since the ice/water system was found to be a system

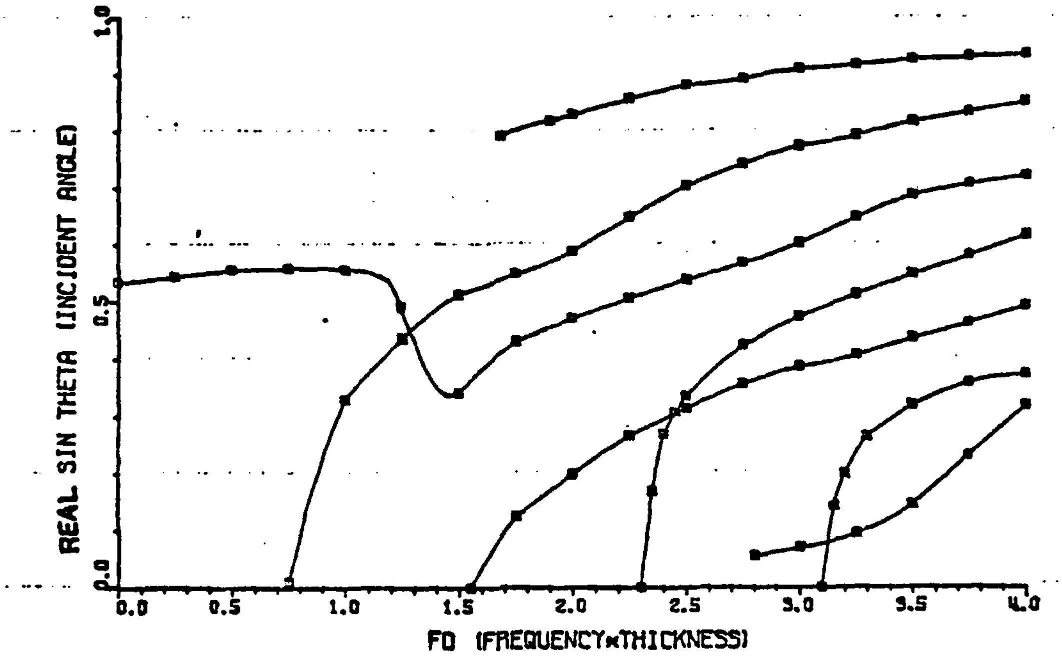

Figure 7. Mode trace for air/ice/water system. Satô values used; $v_d = 3500$ m/s, $v_s = 1550$ m/s, $v_\ell = 1500$ m/s, $v_{air} = 340$ m/s, $\rho_{ice} = .917$, $\rho_{water} = 1.02$, $\rho_{air} = 0.001183$.

where the leaky Rayleigh wave cannot exist, a similar system such as the air/ice/water system could well have differences attributable to this unique situation which does not exist for other air/solid/liquid systems. To check this theory, four different ice densities were used in (13), giving different values for the density ratio of ρ_ℓ/ρ_s. Figure 8 shows the "plateau" from Brower et. al. [9], below which the leaky Rayleigh wave exists, above which it does not, and the four density ratios — two above and two below the "plateau". This change of parameter value was purely of investigative nature since the density-modified "ice" represented not ice at all, but a solid with identical shear and longitudinal wave velocities and different density.

Several changes can be seen in figs. 9-12, which show the solutions to (13) for the four density ratios. The mode that, in fig. 7, had a negative slope now has a positive slope throughout the investigated range. This same mode now approaches asymptotically the Rayleigh wave velocity for this system as predicted by Pitts [8]. The top mode which was discontinuous in fig. 7 is now part of this new positive slope mode. Some problems are still present, however. One mode, in both figs. 9 and 10, has a negative sloped area and is discontinuous. There still are no modes representing the longitudinal wave intercepting the abscissa ($\sin\theta=0$).

D. Adjustment of acoustic impedance.

The acoustic impedance is often important when considering re-

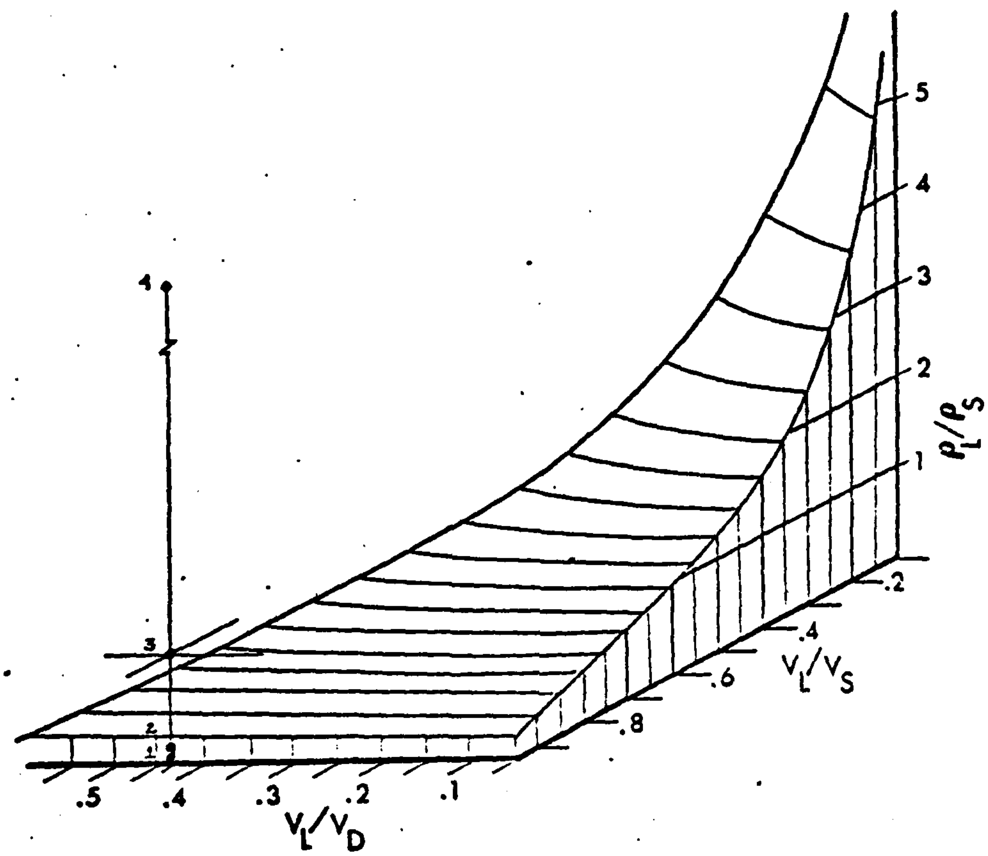

Figure 8. "Plateau" of existence for Rayleigh wave. Points below plateau represent systems where the Rayleigh surface wave does exist, points above represent those where it does not. Point 1 has density ratio of 0.1; point 2, 0.3; point 3, 1.11; point 4, 11.

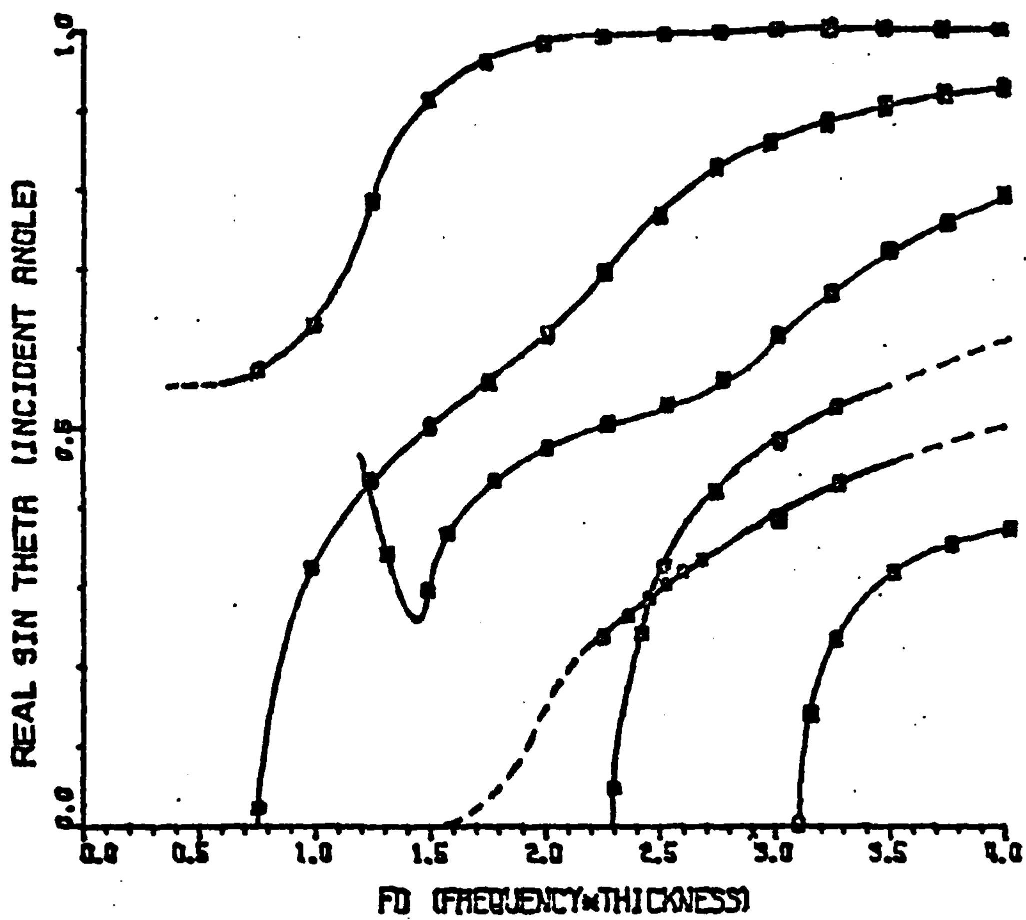

Figure 9. Mode trace for air/ice/water system with modified ice density. Average Sató values used, ρ_{ice}= 10.2. Density ratio of liquid to solid is below "plateau" (ratio=0.1) where leaky Rayleigh exists.

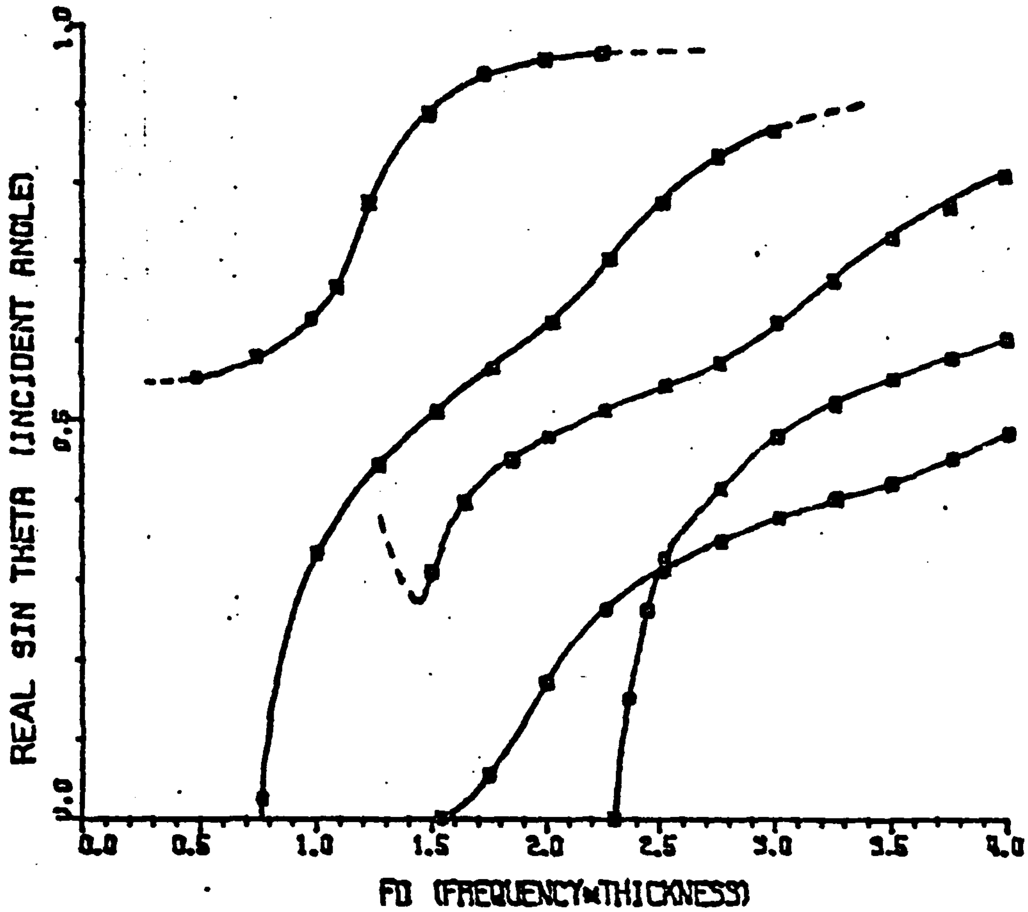

Figure 10. Mcde trace for air/ice/water system with modified ice density. Average Satő values used, ρ_{ice}= 3.06. Density ratio of liquid to solid is below "plateau" (ratio=0.3) where leaky Rayleigh exists.

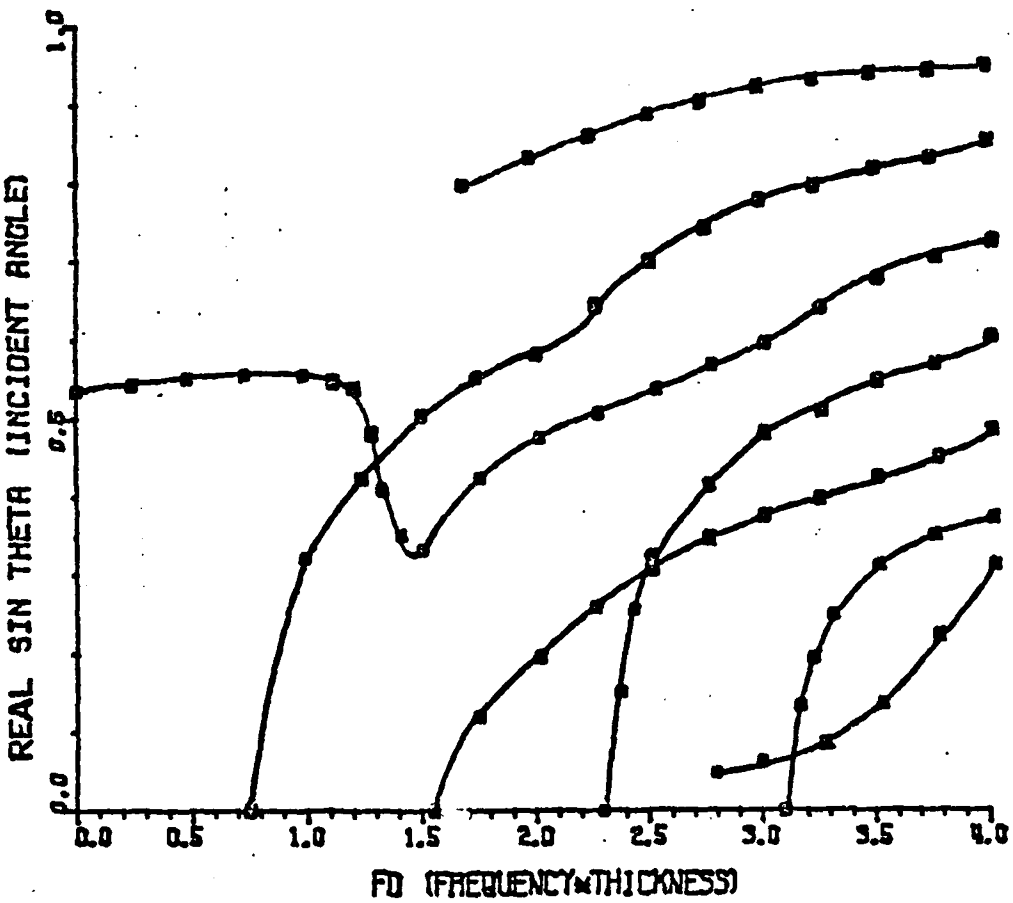

Figure 11. Mode trace for air/ice/water system. Average Satō values used. Density ratio of liquid to solid is above "plateau" (ratio=1.11) where leaky Rayleigh does not exist.

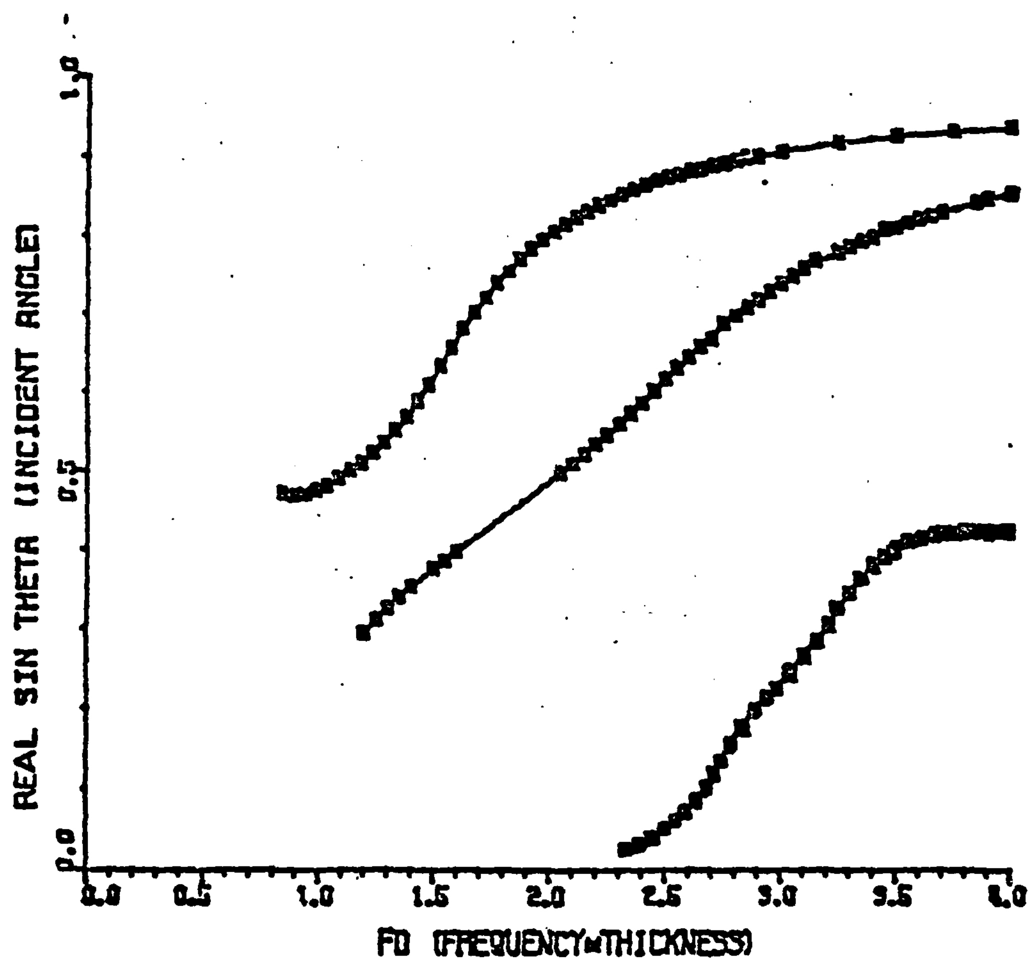

Figure 12. Mode trace for air/ice/water system with modified ice density. Average Satō values used, ρ_{ice} = 0.10. Density ratio of liquid to solid is above "plateau" (ratio=11) where leaky Rayleigh does not exist.

flections from an interface. A matched-impedance system, or one in which the wave velocity times the density of each substance is equal, generally behaves differently than one that is not matched. Again, a hypothesis was made that a matched-impedance system between the ice and water would eliminate the problem of discontinous and negative sloped modes as shown in figs. 7 and 9-12. To consider the hypothetical case of matched impecances of water and ice, the ice density was again changed. Figure 13 shows the solutions to the impedance-matched system, the normal ice/water/air system, and one of the "below plateau" density ratio systems. The impedance-matched system gives results that differ little from the normal system. Specifically, the previously discussed problems are still present, leading one to believe that the relatively small difference in acoustic impedances between ice and water is not the reason discontinuous modes exist.

E. Expansion of continuous-mode range.

The curves located in the area bounded by fd of 1.75 and 4 and sinΘ of 0.2 and 1.0 do not show discontinuities and negative slopes. Due to the frequencies and plate thicknesses commonly used in the laboratory, this area of solutions is the area most often verified by experimentation. For these reasons, (13) was run in the simplex using high, average, and low shear and longitudinal wave velocities for ice (from Satô [10]) in this bounded area, other parameters (density, etc.) being held constant. Shown in figs. 14 and 15 are the

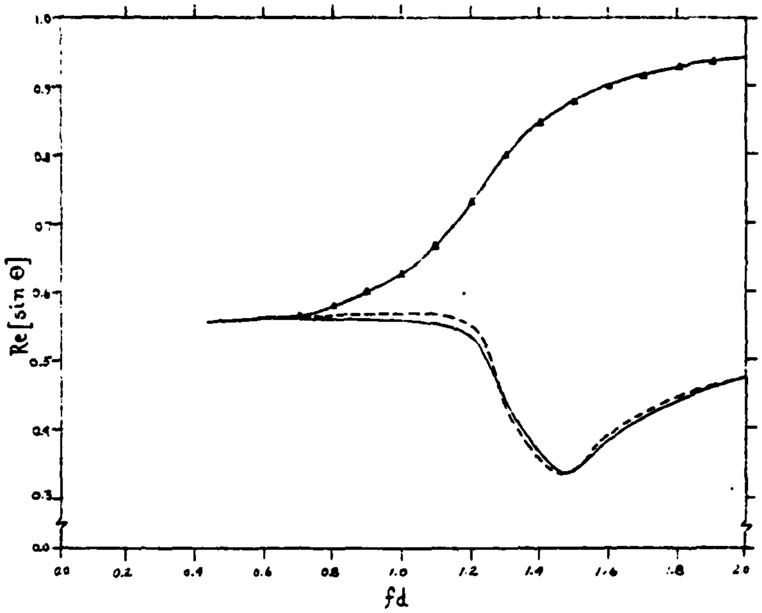

Figure 13. Partial mode trace for air/ice/water system using three different ice densities; actual ice, ρ=0.917 (solid line); impedance-matched ice, ρ=0.987097 (dashed line); and "below plateau" ice, ρ=3.06 (line with triangular points).

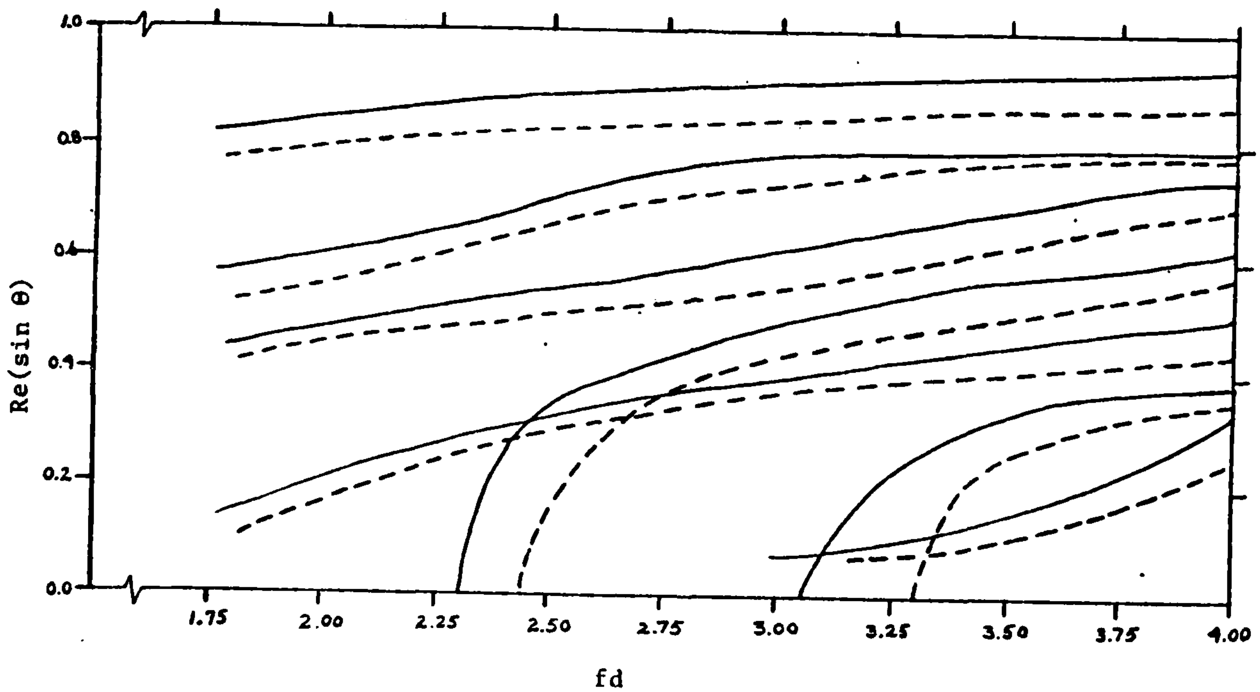

Figure 14. Mode trace of air/ice/water system for Satō average and high values. Average values (denoted by solid lines) are; v_d=3500 m/s, v_s=1550 m/s, v_ℓ=1500 m/s, v_{air}=340 m/s. High values (dashed lines) are; v_d=3600 m/s, v_s=1650 m/s (other values are the same).

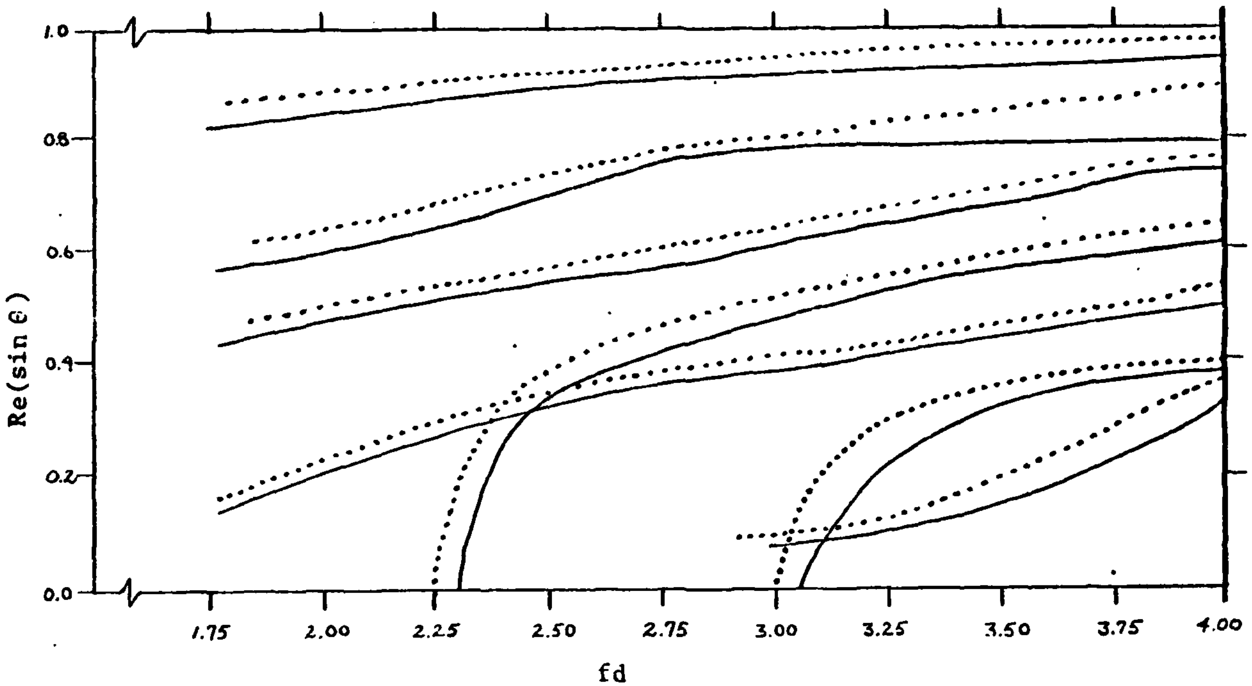

Figure 15. Mode trace of air/ice/water system for Satō average and low values. Average values (denoted by solid lines) are; v_d=3500 m/s, v_s=1550 m/s, v_ℓ=1500 m/s, v_{air}=340 m/s. Low values (dotted lines) are; v_d=3400 m/s, v_s=1500 m/s (other values are the same).

results of these simplex runs. The modes shown are continuous and positive sloped. The shapes of the modes vary only slightly with change in velocity values and remain well-behaved (that is, easily traced) throughout this area.

The variation in spacing of modes in terms of sinθ is primarily a function of fd. Variations in density and velocity parameters for different types of ice are thus of minor importance.

This affords one the opportunity to determine the thickness of the ice by observing at what angles of incidence a plate mode is set up while f is being held constant. This method of determining ice thickness is not easily applicable when fd lies outside the values given above because the mode structure and spacing in other areas of the sinθ versus fd diagrams does depend significantly on the ice density and the values of the sonic velocity in the ice.

F. *Imaginary part of solutions*.

The imaginary parts of the solutions for the sinθ values were calculated throughout the simplex runs for the air/ice/water system (see sample output in Appendix B). Though it is the real part of the sinθ value that is observed experimentally, the imaginary part holds important information. When tracing two crossing modes, the imaginary parts of the solutions distinguish the two modes from one another. This is especially useful when there is a question whether the two modes cross at all, as in the example shown in fig. 16. Ignoring the "traceable"

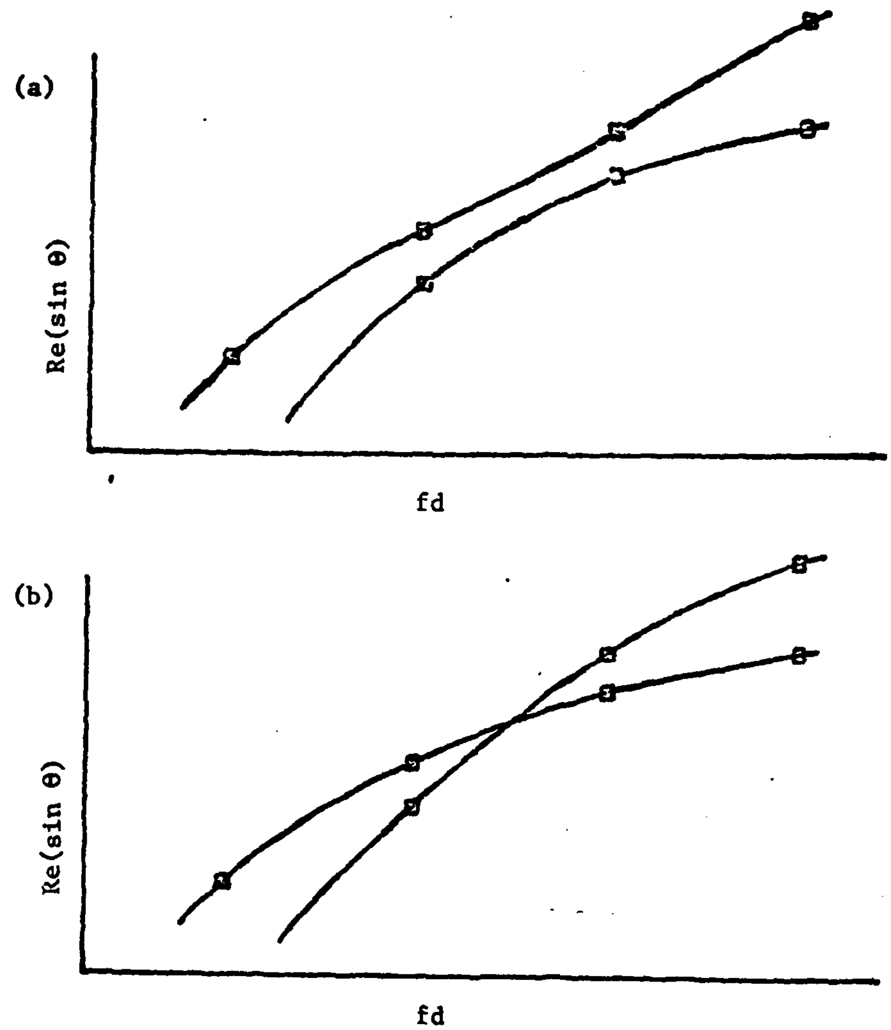

Figure 16. Example of mode trace for modes where crossing is in question. Squares are data points, (a) and (b) are possible choices for mode shapes.

quality of the imaginary part of the solution, fig. 16 (a) or (b) may each be considered equally correct in representing the physical situation.

Pitts [8] has also stated that the magnitude of the imaginary part of the solution indicates whether the zero will be a physical as well as mathematical solution to the system. There has been no determination, however, as to the limits of the magnitude of the imaginary part where this is a factor.

CHAPTER VI

CONCLUSIONS AND SUGGESTIONS FOR FUTURE RESEARCH

Equation (13) represents a complicated function which causes problems with optimization not found in simpler functions such as that represented by (7). Highly varying functional values, portions of modes with negative slope, and discontinuous modes all contribute to the difficulties experienced in solving the equations for air/ice/water system modes.

The simplex, in its modified form, is able to efficiently optimize complicated functions such as (13). With operator intervention (watching imaginary part progression, etc.), the routine can trace modes as well as sample modes of a particular fd. This combination allows complete mode traces for all values of $\sin\Theta$ and fd for two and three substance systems, yielding precise and reproducible results.

Due to repeated use of the subroutine which calculates functional values (on the order of 100 to 500 times per data point), the program should be run on a computer with direct access to the central processing unit (such as the DEC PDP-MINC 11) or one which has optional use of virtual memory, thus cutting computation costs by as much as 90%.

By actual runs, the water/brass/water system results of Pitts [8] have been confirmed. Some of the calculated results of the air/ice/water system have been verified qualitatively only. Preliminary lab-

oratory runs suggest the calculated modes are correct. Due to problems with experimental set-up, determination of actual parameters, and recording of data, insufficient verification has resulted from the laboratory. Figure 17 shows the theoretical trace of the average Sató parameter values for air/ice/water and two experimental points. The frequency used was 1.84 MHz, plate thickness was approximately 1 mm (melting of ice prevented precise measurement), giving an fd of approximately 1.8. Due to constraints in transducer housing and set-up, only angles between 15° and 60° could be viewed. Two non-specular reflections were observed, at 26° and 37°, giving the two points shown in fig. 17. Given the uncertainty in the actual parameters of the system and the experimental problems, the points correspond well with the calculated values.

Future research should include continued confirmation of calculated solutions to the air/ice/water system. Methods for precise determination of actual parameter values such as shear and longitudinal wave velocities should be pursued. Though Negishi [22] has recently reported on negative group velocities, this area should be investigated to confirm or deny the existence of this phenomenon. Pitts has recently done research on systems of water/aluminum in which negative slopes occur in the mode traces. The mere presence of a negative slope may or may not indicate the existence of unusual propagation characteristics.

A functional basis should be found to explain discontinuous modes.

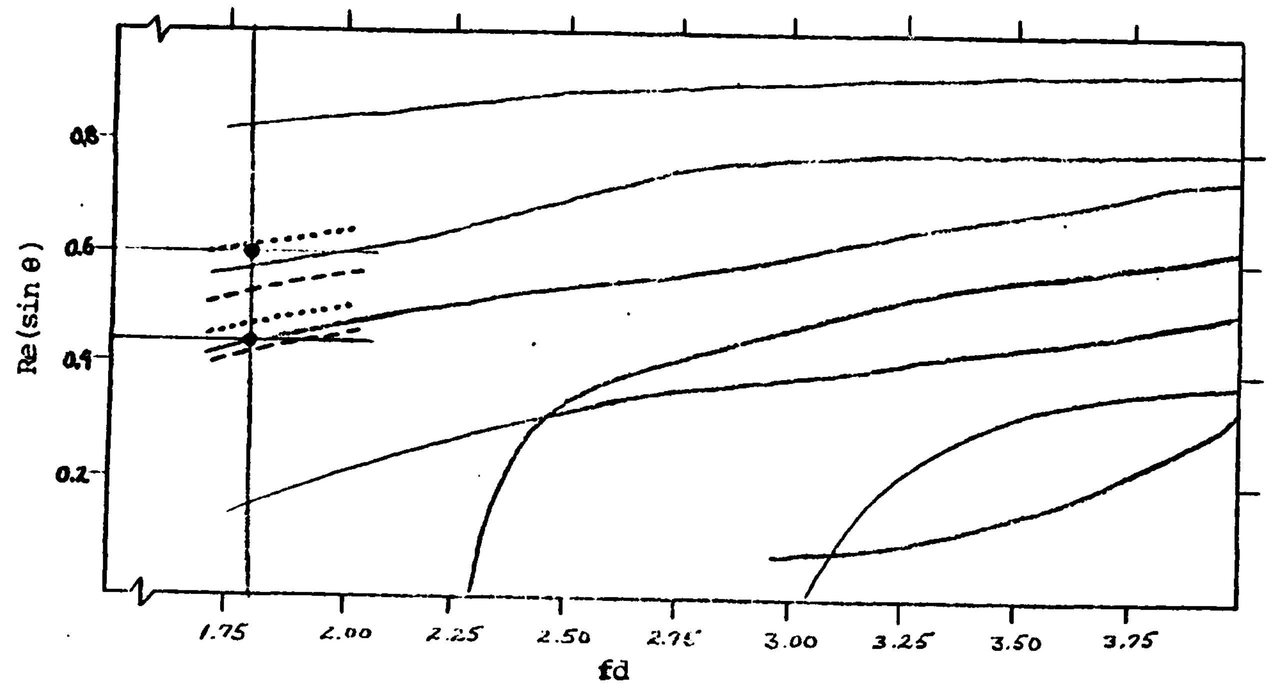

Figure 17. Simplex mode trace of Satō average values for air/ice/water system showing two experimental points at $fd = 1.8$, and $\sin \theta = 0.44$ and 0.6 (26° and 37°). Theoretical limits are given by dotted lines (Satō low values) and dashed lines (Satō high values) for y-axis uncertainty, and limits for x-axis uncertainty are unknown due to undetermined change in ice thickness (melting).

Though no physical reason is apparent for such discontinuities, these modes may be the "missing" intercepts representing the longitudinal wave.

Should the modes in figs. 14 and 15 be confirmed by experimentation, they will be valuable in practical applications such as sonar, non-destructive testing, and seismic studies. The simplex will then have proven to be a fast, efficient method of determining solutions to the air/ice/water system, as well as any other similar system consisting of a gas-solid-liquid layered structure.

APPENDICES

A. Simplex FORTRAN IV computer program in mode-trace form. Air/Ice/Water system reflection coefficient for simplex subroutine.

```
C      ****************************************************************
C      *****      SIMPLEX CPTIMIZING PROGRAM — LINEAR PROGRAMMING      **
C      ****************************************************************
C               CRIGINAL WORK CCNE EY HUANG ANC ERCWER
C               REVISEC BY NG ANC FIMBERGER, AUG78
C
C               FURTHER REVISEC BY FIMBEFGER, SEPT. 78-APRIL 79
C
C      THIS FCRM CF SIMPLEX TRACES A MCDE FRCM FC=C TC FC=4.0
C      OTHER FORMS SCAN A PARTICLLAR FC FROM SIN THETA=C TC 1.0
C
C      THE VARIABLE ARRAY LFLAG IS SET UP TC INCICATE THE CRCER
C      IN WHICH THE SIMPLEX METHCD REACHES ITS FINAL ANSWER —
C         1, A REFLECTICN HAS OCCLRREC
C         2, A CONTRACTICN HAS CCCLRRED
C         3, A NEW MINIMLM WAS NOT REACHEC
C         4, A PARAMETER REPLACEMENT
C         5, AN EXPANSICN OCCLRREC
C         6, A FAILEC CCNTRACTION
C
C       THE PCINTS AT WHICH THESE ARE PRINTEC IN THE PROGRAM IS A GOOD
C           INDICATICN OF WHAT THE VARICUS BRANCHES ARE CCING
C
C      aaaaaaaaaaaaaaaaa  A BASIC VERSION CF THIS PROGRAM HAS ALSO
C      aaaaaaaaaaaaaaaaa  BEEN WRITEN — WANG SPECIAL FLNCTICNS USEC
C
C           #####     SEE NELDER AND MEAC REFERENCE IN M.S. THESIS
C           #####     OF HIMBERGER FOR DETAILS CN SIMPLEX
C
       DIMENSION X1(2),PARM(2,3),FMIN(3),CENT(2)
       DIMENSION XR(2),XC(2),XE(2)
       DIMENSION LFLAG(5CO)
C      <<<<<  THE ARRAY SP RETAINS THE LAST ITTERATED VALUE TC
C      <<<<<  CHECK AGAINST THE PRESENT CNE — FCR TRACING MCDES
       DIMENSION SP(5C)
       INTEGER K
       INTEGER L
       C=1
       FD=4.C5
       W=1
       SP(W)=C.19781
     1 FD=FD-C.C5
       IF(FC.LT.1.75) GC TO 5C0
       B=SP(W)
       GO TO 3
     2 B=B+C.C1
       IF(B.GT.(SP(1)+0.10)) GO TO 1
     3 L=C
C      *****  X1(1) IS THE STARTING REAL SIN GUESS
C      *****  AND X1(2) IS THE IMAGINARY SIN GUESS
       X1(1)=B
       X1(2)=-0.01
C      *****  ST1 AND ST2 ARE THE INCREMENTAL VALUES THE SIMPLEX
C      *****  USES TC FORM THE 'SIMPLEX' ITSELF
       ST1=0.C01
       ST2=-C.C01
       K=0
C      *****  THE ARRAY 'PARM' HCLDS THE PCINTS THEMSELVES
       PARM(1,1)=X1(1)
```

```
      PARM(1,2)=X1(1)+ST1
      PARM(2,1)=X1(2)
      PARM(2,2)=X1(2)
      PARM(1,3)=X1(1)
      PARM(2,3)=X1(2)+ST2
    5 CONTINUE
      DO 20 I=1,3
      DO 10 J=1,2
   10 X1(J)=PARM(J,I)
C     *****  THE SUBROUTINE IS CALLED UPON REPEATEDLY TO FIND
C     *****  THE FUNCTIONAL VALUE OF THE VARIOUS POINTS IN THE SIMPLEX
      CALL FUNCT(X1,F1,FO,K,&166)
   15 FMIN(I)=F1
   20 CONTINUE
   25 I1=1
      I2=1
      I3=1
      DO 30 I=2,3
      IF(FMIN(I1).LT.FMIN(I)) I1=I
   30 CONTINUE
      DO 35 I=1,2
   35 CENT(I)=0.
      DO 45 I=1,3
      IF(I.EQ.I1) GO TO 45
      DO 40 J=1,2
   40 CENT(J)=CENT(J)+PARM(J,I)
      IF (FMIN(I2).GT.FMIN(I)) GO TO 41
      I3=I2
      I2=I
      GO TO 45
   41 I3=I
   45 CONTINUE
      DO 50 I=1,2
   50 CENT(I)=CENT(I)/2.0
C     **********  THE 'CRITER' IS THE CRITERION USED TO DETERMINE
C     **********  THE POINT AT WHICH THE SIMPLEX HAS ITERATED
C     **********  CLOSELY ENOUGH  TO WHAT HAS BEEN CALLED 'ZERO'
      CRITER=1.0E-06
      POLE=0.
C     $$$$$$$$$$$  THE SIMPLEX ACTUALLY 'FALLS UPON' ITSELF
C     $$$$$$$$$$$  OR COLLAPSES -- WHEN THE DISTANCE BETWEEN
C     $$$$$$$$$$$  THE POINTS OF THE 'SIMPLEX' IS < THE CRITER,
C     $$$$$$$$$$$  YOU HAVE REACHED A ''ZERO''.  NOTE THAT THIS
C     $$$$$$$$$$$  ''ZERO'' MAY NOT BE IDENTICALLY  EQUAL TO 0
C     $$$$$$$$$$$  IN FACT, IF IT IS APPROX. ZERO, IT MAY BE ONLY
C     $$$$$$$$$$$  A LOCAL MINIMUM -- NOT PART OF THE MODE STRUCTURE
      DO 60 I=1,3
      POLE=POLE+(FMIN(I)-FMIN(I3))**2
   60 CONTINUE
      POLE=SQRT(POLE/2.0)
      IF(POLE.LE.CRITER) GO TO 160
      DO 85 I=1,2
      XR(I)=2.*CENT(I)-PARM(I,I1)
   85 X1(I)=XR(I)
      L=L+1
C     $$$$$$$$$$$$$$$$$$     REFLECTION     $$$$$$$$$$$$$$$$$$$$$
      LFLAG(L)=1
      CALL FUNCT(X1,FR,FO,K,&166)
      IF(FMIN(I2).GE.FR.AND.FR.GE.FMIN(I3)) GO TO 130
```

```
      IF(FR.LT.FMIN(I3)) GO TO 140
      IF(FMIN(I1).GT.FR.AND.FR.GT.FMIN(I2)) GO TO 95
      DO 90 I=1,2
      XC(I)=0.5*PARM(I,I1)+0.5*CENT(I)
   90 X1(I)=XC(I)
      L=L+1
C     $$$$$$$$$$$$$$$$$$     CONTRACTION     $$$$$$$$$$$$$$$$$$$
      LFLAG(L)=2
      CALL FUNCT(X1,FC,FD,K,&166)
      GO TO 105
   95 L=L+1
C     $$$$$$$$$$$$$$$$$$     NO NEW MINIMUM     $$$$$$$$$$$$$$$$
      LFLAG(L)=3
      DO 100 I=1,2
      PARM(I,I1)=XR(I)
      XC(I)=.5*PARM(I,I1)+.5*CENT(I)
  100 X1(I)=XC(I)
      CALL FUNCT(X1,FC,FD,K,&166)
  105 IF(FMIN(I1).GT.FC) GO TO 120
      L=L+1
C     $$$$$$$$$$$$$$$$$$     REPL. PARAM.     $$$$$$$$$$$$$$$$$$
      LFLAG(L)=4
      DO 115 I=1,3
      DO 110 J=1,2
  110 PARM(J,I)=0.5*(PARM(J,I)+PARM(J,I3))
  115 CONTINUE
      GO TO 5
  120 DO 125 I=1,2
      X1(I)=XC(I)
  125 PARM(I,I1)=XC(I)
      FMIN(I1)=FC
      GO TO 155
  130 DO 135 I=1,2
      X1(I)=XR(I)
  135 PARM(I,I1)=XR(I)
      FMIN(I1)=FR
      GO TO 155
  140 CONTINUE
      DO 145 I=1,2
      XE(I)=2.*XR(I)-CENT(I)
  145 X1(I)=XE(I)
      CALL FUNCT(X1,FE,FD,K,&166)
      IF(FMIN(I3).LE.FE) GO TO 156
      L=L+1
C     $$$$$$$$$$$$$$$$$$     EXPANSION     $$$$$$$$$$$$$$$$$$$$$
      LFLAG(L)=5
      DO 150 I=1,2
      X1(I)=XE(I)
  150 PARM(I,I1)=XE(I)
      FMIN(I1)=FE
  155 CONTINUE
      GO TO 25
  156 L=L+1
C     $$$$$$$$$$$$$$$$$$     FAILED CONTRACTION     $$$$$$$$$$$$
      LFLAG(L)=6
      GO TO 130
C     $$$$$  THE LFLAG ARRAY HAS NOT BEEN PRINTED OUT IN THIS FORM
C     $$$$$  OF THE SIMPLEX ROUTINE TO SAVE I/O TIME
C     <<<<<  THIS ROUTINE CHECKS TO SEE IF INITIAL ZERO IS AT CORRECT
```

```
C     <<<<<  STARTING PCINT -- AGAIN FOR MODE TRACING  >>>>>
  160 IF(G.NE.1.C) GO TO 161
      IF(PARM(1,I3).LT.C.180.OR.PARM(1,I3).GT.C.220) GC TO 167
      W=2
      SP(W)=PARM(1,I3)
      WRITE(6,185) (PARM(J,I3),J=1,2)
      WRITE(6,190) FMIN(I3),K,FC,B
      G=G+1
      GC TC 1
C     <<<<<  THIS ROUTINE IS USED FOR CHECKING TO SEE IF SAME MODE
C     <<<<<  HAS BEEN FOUND - IF NOT, IT DISCCUNTS IT AND TRIES AGAIN
  161 CONTINUE
      IF(PARM(1,I3).GT.(SP(W)+0.01).OR.PARM(1,I3).LT.(SP(W)-0.03))
     1GC TC 162
      WRITE(6,185) (PARM(J,I3),J=1,2)
      WRITE(6,190) FMIN(I3),K,FC,B
      W=W+1
      SP(W)=PARM(1,I3)
      G=G+1
      GO TO 1
  162 WRITE(6,200) FC,FMIN(I3),B,(PARM(J,I3),J=1,2)
      IF(G.EQ.1.0) GC TC 2
      GC TC 2
  166 IF(G.EQ.1.0) GC TC 169
      IF(PARM(1,I3).GT.(SP(W)+C.01).OR.PARM(1,I3).LT.(SP(W)-0.03))
     1GO TO 162
      WRITE(6,193) FMIN(I3),FD,B,(PARM(J,I3),J=1,2)
      W=W+1
      SP(W)=PARM(1,I3)
      G=G+1
  167 IF(G.EQ.1.0) GC TO 2
  168 GO TO 1
  169 WRITE(6,194)
      GC TC 160
C                                   FORMAT SECTION
  185 FORMAT(///' FINAL PARAMETER VALUES - REAL AND IMAG. PARTS OF SIN'
     1/(2E15.6))
  190 FORMAT(/,' FUNCTION VALUE=',E15.6,' 4 ITER=',I7,' FD=',F6.2,
     C' B=',E15.6)
  193 FORMAT(/,' NC AFTER 300 ITER.',E15.6,' = FUNCT. VALUE',
     1/' FD=',F6.2,' B=',E15.6,/,' PARAM. VALUES REACHED=',/,(2E15.6))
  194 FORMAT(/,' FINDING FIRST POLE-NOT CONVERGENT, CONTINUING')
  199 CONTINUE
  200 FORMAT(//' PARAM. VAL. NOT WITHIN LIMITS OF PREVIOUS VAL.',
     1/,' FD=',F6.2,' FUNCT. VAL.=',E15.6,' B=',E15.6,/,
     1' PARAMETER VALUES=',(2E15.6))
  310 CONTINUE
  500 STOP
      END
      SUBROUTINE FUNCT(X1,F1,FD,K,*)
C       SUBROUTINE FOR NUMERATOR OF WANG'S REFLECTION COEFFICIENT
C          FOR WATER/ICE/AIR
C          #######  LOW VALUES FOR VS AND VL USED  ######
      INTEGER K
      DIMENSION X1(2)
      COMPLEX A,C,E,G,H,Q,R,S,T,C1,ANG
      COMPLEX SYM,ASY,Z3,Z1,CC,EL,GD,DCW
      COMPLEX NUM
      COMPLEX Y1,Y3
```

```
      U1=X1(1)
      U2=X1(2)
      ANG=CMPLX(U1,U2)
      DEN1=1.02
      DEN3=0.001183
      DENP=0.917
      V1=1.5
      V3=0.34
      VD=3.4
      VS=1.5
      C1=(0.000,1.000)
      P=3.1415926*F0/V1
      A=(VS/V1)*ANG
      C=(1.0-2.0*(A**2))**2
      E=CSQRT((V1/VD)**2-(ANG**2))
      G=CSQRT((V1/VS)**2-(ANG**2))
      H=4.000*((VS/V1)**4)*(ANG**2)*E*G
      Q=CSIN(P*E)
      R=CCOS(P*E)
      S=CSIN(P*G)
      T=CCOS(P*G)
      SYM=C*R*S+H*Q*T
      ASY=C*Q*T+H*R*S
      Y3=CSQRT((V1/V3)**2-(ANG**2))
      Y1=CSQRT(1-(ANG**2))
      Z3=C1*(DEN3/DENP)*(E/Y3)
      Z1=C1*(DEN1/DENP)*(E/Y1)
      GC=Z1*R*T
      GU=2.000*(SYM-(Z3*Q*S))
      GD=(C*S*T)+(H*Q*R)
      DOW=GU*(ASY+GC)-(Z1-Z3)*GD
      NUM=GU*(ASY-GC)+(Z1+Z3)*GD
      G7=REAL(NUM)
      G8=AIMAG(NUM)
      F1=ABS(G7)+ABS(G8)
      K=K+1
      IF(K.LE.300) GO TO 10
      RETURN 1
   10 RETURN
      END
```

B. Sample simplex output for mode-trace form. Shown are points that iterate to a solution to the reflection coefficient, points that do not converge within a set number of times but give intermediate values, and points that do not belong to the traced mode but were given during the course of the iteration for additional information.

```
FINAL PARAMETER VALUES - REAL AND IMAG. PARTS OF SIN
  0.318198E 00  -0.141639E-01

FUNCTION VALUE=   0.149012E-07 # ITER=    125 FD=  3.75
B=   0.326468E 00

NC AFTER 300 ITER.   0.134110E-06 = FUNCT. VALUE
FD=  3.70 B=   0.318198E 00
PARAM. VALUES REACHED=
  0.308662E 00  -0.128520E-01

NC AFTER 300 ITER.   0.894070E-07 = FUNCT. VALUE
FD=  3.65 B=   0.308662E 00
PARAM. VALUES REACHED=
  0.297508E 00  -0.113176E-01


FINAL PARAMETER VALUES - REAL AND IMAG. PARTS OF SIN
  0.284263E 00  -0.959546E-02

FUNCTION VALUE=   0.286847E-06 # ITER=     96 FD=  3.60
B=   0.297508E 00

FINAL PARAMETER VALUES - REAL AND IMAG. PARTS OF SIN
  0.268258E 00  -0.774238E-02

FUNCTION VALUE=   0.186265E-07 # ITER=    109 FD=  3.55
B=   0.284263E 00

FINAL PARAMETER VALUES - REAL AND IMAG. PARTS OF SIN
  0.248497E 00  -0.583842E-02

FUNCTION VALUE=   0.447035E-07 # ITER=     96 FD=  3.50
B=   0.268258E 00

NC AFTER 300 ITER.   0.175554E-06 = FUNCT. VALUE
FD=  3.45 B=   0.248497E 00
PARAM. VALUES REACHED=
  0.223357E 00  -0.398661E-02

PARAM. VAL. NOT WITHIN LIMITS OF PREVIOUS VAL.
FD=  3.40 FUNCT. VAL.=   0.558794E-07 B=   0.223357E 00
PARAMETER VALUES=   0.189763E 00  -0.231284E-02
```

C. Sample simplex output for scan form with indicator 'flags'. Descriptions of flags are included in FORTRAN IV program, appendix A.

```
FINAL PARAMETER VALUES - REAL AND IMAG. PARTS OF SIN
  0.435409E 00  -0.169694E 00

FUNCTION VALUE=   0.782311E-07 # ITER=     182 FD=  1.-30 B=   0.759999E 00
15151515151515151515151511211212121121212112121612161212121515151515151515151515151515112
1212115115161612131211212121612121213121212161212121212121312161212121212131212
12121616124112412000000000000000000000000000000000000000000000000000000000000000
00000000000000000000000000000000000000000000000000000000000000000000000000000000
00000000000000000000000000000000000000000000000000000000000000000000000000000000
00000000000000000000000000000000000000000000000000000000000000000000000000000000
00000000000000000000000000000000000000000000000000000000000000000000000000000000
0000000000000000000000000

NC AFT. 1000 ITER.   0.227243E-06 = FUNCT. VALUE
FD=  1.30 B=   0.769999E 00
PARAM. VALUES REACHED=
  0.435410E 00  -0.169694E 00


FINAL PARAMETER VALUES - REAL AND IMAG. PARTS OF SIN
  0.435409E 00  -0.169694E 00

FUNCTION VALUE=   0.208616E-06 # ITER=     150 FD=  1.30 B=   0.779999E 00
1515151151515151515151511212121216161161215121216121515115131611512121212121212
1213121212121121212131212161212121216121212416124121212412410000000000000000000
00000000000000000000000000000000000000000000000000000000000000000000000000000000
00000000000000000000000000000000000000000000000000000000000000000000000000000000
00000000000000000000000000000000000000000000000000000000000000000000000000000000
00000000000000000000000000000000000000000000000000000000000000000000000000000000
00000000000000000000000000000000000000000000000000000000000000000000000000000000
0000000000000000000000000
```

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